Ethyl 2-ethyl-3-hydroxybutanoate 5465-11-2 | DTXSID90282959

Model Performance

Model	Data
Model	Dala

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 1.63

Global applicability domain: Inside

Local applicability domain index: 5.57e-01

Confidence level: 6.97e-01

Nearest Neighbors from the Training Set

Image not found

Isobutyl acetate Measured: 1.78 Predicted: 1.82 Image not found

3-Methylbutyl acetate Measured: 2.25 Predicted: 2.20 Image not found

Methyl 6-oxoheptanoate Measured: 0.55 Predicted: 8.61e-01

Image not found

Butan-2-yl acetate Measured: 1.72 Predicted: 1.85 Image not found

Methyl pivalate
Measured: 1.83
Predicted: 1.76